REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
03-06-2016	Final Report	1-Nov-2012 - 31-Oct-2015

4. TITLE AND SUBTITLE
Final Report: Statistical Multiscale Property Metrics for Nanorod and Nanoplatelet Composite Membranes and Films

5a. CONTRACT NUMBER
W911NF-13-1-0013

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

6. AUTHORS
Peter Mucha, Feng (Bill) Shi, Simi Wang, Ruhai Zhou, M. Gregory Forest

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
University of North Carolina - Chapel Hill
104 Airport Drive, CB 1350
Suite 2200
Chapel Hill, NC 27599 -1350

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
60317-MS.13

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
This proposal outlines a strategy to construct statistical multiscale metrics for nano-rod and nano-platelet films and membranes, integrating over the processing-to-property pipeline. We first identify and model the sources of randomness and uncertainty. Next we describe our existing probabilistic tools and results for hydrodynamic processing of nano-rod and nano-platelet membranes and films. These previous results provide statistical databases, and the means to generate data on demand for flow-processed nano-rod films and membranes; the

15. SUBJECT TERMS
Network Graph Theory, Community Detection, Percolation, Property Distributions

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Mark Forest
UU	UU	UU	UU		19b. TELEPHONE NUMBER
					919-962-9606

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

Report Title

Final Report: Statistical Multiscale Property Metrics for Nanorod and Nanoplatelet Composite Membranes and Films

ABSTRACT

This proposal outlines a strategy to construct statistical multiscale metrics for nano-rod and nano-platelet films and membranes, integrating over the processing-to-property pipeline. We first identify and model the sources of randomness and uncertainty. Next we describe our existing probabilistic tools and results for hydrodynamic processing of nano-rod and nano-platelet membranes and films. These previous results provide statistical databases, and the means to generate data on demand for flow-processed nano-rod films and membranes; the purpose of the proposed effort is that existing property metrics for these material systems have been wholly inadequate except near percolation thresholds for isotropic rod dispersions. In response, we propose a new bridge between flow-processing statistical databases and property metrics in the form of network graphs. Spectral graph analysis and computation generate bulk-to-particle scale properties, while sufficient realizations give robust property statistics.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
09/02/2014	8	Feng Shi, Simi Wang, M. Gregory Forest, Peter J. Mucha, Ruhai Zhou. Network-Based Assessments of Percolation-Induced Current Distributions in Sheared Rod Macromolecular Dispersions, Multiscale Modeling & Simulation, (03 2014): 0. doi: 10.1137/130926390
09/02/2014	9	John Mellnik, Paula A. Vasquez, Scott A. McKinley, Jacob Witten, David B. Hill, M. Gregory Forest. Micro-heterogeneity metrics for diffusion in soft matter, Soft Matter, (08 2014): 0. doi: 10.1039/C4SM00676C

TOTAL: 2

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received	Paper

TOTAL: 4

Number of Papers published in non peer-reviewed journals:

(c) Presentations

- 2012, The Dissipative Side of Fluctuation-Dissipation in Soft Matter, tutorial plenary for SAMSI Workshop on Nonlocal Continuum Models for Diffusion, Mechanics, and Other Applications, SAMSI, Research Triangle, NC, June 25
- 2012, Nematics near and far from equilibrium, SIAM Annual Meeting, Minneapolis, MN, Minisymposium on Mathematics & Mechanics of Soft Matter, Organizers: Raffaella De Vita & Paolo Biscari, July 11
- 2012, Active nematic flows, American Physical Society-Division of Fluid Dynamics Annual Meeting, San Diego, CA, Mini-Symposium in Memory of Daniel D. Joseph, Organizer: Howard Hu, November 19
- 2013, Defects in nematic polymer hydrodynamics, Isaac Newton Institute, Cambridge University, Mathematics of Liquid Crystals Program, Workshop on Symmetry, Bifurcation and Order Parameters, January 9
- 2013, Mathematical and Numerical Challenges in Living Biological Materials, International Conference on Numerical Analysis and Applied Mathematics, Rhodes, Greece, plenary, September 24
- 2014, Nematic polymer hydrodynamics, Arizona Program in Applied Mathematics 35th Anniversary Workshop, Tucson, AZ, April 26
- 2014, Active nano-rod dispersions, SIAM Annual Meeting, mini-symposium on Nonlinear Fluids, S. Walker and A. Salgado, organizers, Chicago, IL, July 8
- 2014, Nano-rod dispersion flows and induced material properties, AFOSR Computational Mathematics annual meeting, Arlington, VA, July 29
- 2015, Computational challenges in complex biological fluids, Tulane University, Scientific Computing around Louisiana workshop, plenary, March 21
- 2015, Data-Driven Modeling of Living Fluids, Department of Mathematics, Applied Mathematics & Statistics, Case Western Reserve, Cleveland, OH, April 13
- 2015, Dynamic Organization of the Yeast Genome, Institute for Nonlinear Science, Shanghai Xiao Tong University, Shanghai, China, June 12
- 2015, Modeling the physical structure and function of living biological soft matter, Pacifichem 2015, Session on The Physical Structure & Function of Biological and Bioinspired Soft Matter, Honolulu, Hawaii, Dec 16
- 2016, Dynamic Organization of DNA in Living Yeast, Lecture 1 (Colloquium) of the Magnus Lectures, Department of Mathematics, Colorado State University, April 4

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Fellow of the Society for Industrial and Applied Mathematics, 2012

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Samuel Heroy	0.75	
FTE Equivalent:	**0.75**	
Total Number:	**1**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Greg Forest	0.08	
Peter Mucha	0.08	
FTE Equivalent:	**0.16**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Our group has continued to develop network graph representations and community detection methods on numerical realizations of nanorod dispersions. The focus of this effort is the
mechanism of mechanical percolation, where we are developing multiscale rigidity cascades in the nanorod phase. Forest with collaborators at South Carolina and Old Dominion have generalized our hydrodynamic codes to activity at the nanorod scale, applicable to catalytic nanorods in a reactive solvent. A recent publication in Soft Matter of the Forest group develops tools to detect heterogeneity at the microscale from microbead tracking experimental data, while another paper in the Journal of the American Statistical Association develops Bayesian methods to rank models for microbead rheology on the basis of experimental data. A paper that just appeared online in the journal Entropy builds a theoretical framework for active fluid models at kinetic to macroscopic scales. A paper that just appeared online in Nucleic Acids Research shows how entropic polymeric modeling can explain much of the dynamics and organization of chromosomes in living cells. The publications are all uploaded into the ARO website, with the most recent ones being:

Microheterogeneity metrics for diffusion in soft matter, J. Mellnik, P. Vasquez, S. McKinley, J. Witten, D. Hill, M.G. Forest, Soft Matter 10, 7781-7796 (2014)

Structure formation in sheared polymer-rod nano-composites, G. Ji, Q. Wang, MG Forest, Discrete and Continuous Dynamical Systems B, 8(2) (2015)

Kinetic attractor phase diagrams of active nematic suspensions: the dilute regime, M.G. Forest, R. Zhou, Q. Wang, Soft Matter 11(32): 6393-402 (2015) DOI: 10.1039/c5sm00852b

Model comparison and assessment for single particle tracking in biological fluids, M. Lysy, N. Pillai, D.B. Hill, M.G. Forest, J. Mellnik, P. Vasquez, S.A. McKinley, Journal of the American Statistical Association, accepted Jan 22, 2016, to appear

Maximum likelihood estimation for single particle, passive microrheology data with drift, J. Mellnik, M. Lysy, N. Pillai, S. McKinley, J. Cribb, D. Hill, P. Vasquez, M.G. Forest, Journal of Rheology 60, 379 (2016); doi: 10.1122/1.4943988

Hydrodynamic Theories for Flows of Active Liquid Crystals and the Generalized Onsager Principle, X. Yang, J. Li, M.G. Forest, Q. Wang, Entropy 18, 202; special issue on Recent Advances in Non-Equilibrium Statistical Mechanics and Its Applications, Guest Editor Giorgio Sonnino, doi:10.3390/e18060202

Entropy gives rise to topologically associating domains, P. Vasquez, C. Hult, J. Lawrimore, D. Adalsteinsson, M.G. Forest, K. Bloom, Nucleic Acids Research (2016), doi: 10.1093/nar/gkw510

Technology Transfer